Entropy accumulation near quantum critical points: effects beyond hyperscaling

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Abstract. Entropy accumulation near a quantum critical point was expected based on general scaling arguments, and has recently been explicitly observed. We explore this issue further in two canonical models for quantum criticality, with particular attention paid to the potential effects beyond hyperscaling. In the case of a one-dimensional transverse field Ising model, we derive the specific scaling form of the free energy. It follows from this scaling form that the singular temperature dependence at the critical field has a vanishing prefactor but the singular field dependence at zero temperature is realized. For the spin-density-wave model above its upper critical dimension, we show that the dangerously irrelevant quartic coupling comes into the free energy in a delicate way but in the end yields only subleading contributions beyond hyperscaling. We conclude that entropy accumulation near quantum critical point is a robust property of both models.

1. Introduction

Quantum critical points (QCPs) have been extensively studied in heavy fermion metals and related systems [1]. They occur as a non-thermal control parameter is tuned to a second-order phase transition at zero temperature. For thermodynamics, it was shown [2] based on scaling considerations that the thermal expansion [$\alpha = (1/V)(\partial V/\partial T)_{p,N} \propto \partial S/\partial p$, the variation of entropy S with pressure p] is more singular than the specific heat [$c_p = (T/N)(\partial S/\partial T)_p$], in the general case when the tuning parameter is linearly coupled to pressure. Correspondingly, the Grüneisen ratio, $\Gamma = \alpha/c_p$, diverges at the QCP, and the entropy is maximized. The same conclusions apply to a field-tuned QCP, where the magnetic Grüneisen ratio is the magnetocaloric effect. The predicted divergence of the Grüneisen ratio is by now widely observed in quantum critical heavy-fermion metals [3, 4], and the entropy enhancement has recently been explicitly observed in a quantum critical ruthenate [5].

The scaling arguments proceed as follows. Near a QCP, the critical part of the free energy takes the hyperscaling form $F = F_0 T^{d/z+1} f(r/T^{1/(\nu z)})$, where $r = p - p_c$, d is the spatial dimension and ν, z are respectively the correlation-length and dynamic exponents. The universal function $f(x)$ has different asymptotic behaviors in the $x \to 0$ and $x \to \pm\infty$ limits, respectively corresponding to the quantum critical and quantum disordered/renormalized classical regimes. The divergence of Γ can be readily derived, in universal forms as $1/r$ for $|r| \gg T$ and as $1/T^{1/\nu z}$ for $|r| \ll T$ [2]. The $1/r$ divergence in the low-temperature limit also amounts to a sign change of Γ across the QCP. As seen in Fig. 1, this corresponds to an entropy maximization at the QCP

in the low-temperature limit. The extension of this sign change to the finite temperature phase transitions has also been discussed [6].

The hyperscaling form for the free energy is based on the existence of a single critical energy scale, *i.e.*, the gap for the quantum critical excitations $\Delta \sim r^{\nu z}$. In this paper we explore how the scaling form of the free energy arises in some specific models for QCPs, paying particular attention to the possible effects that go beyond hyperscaling.

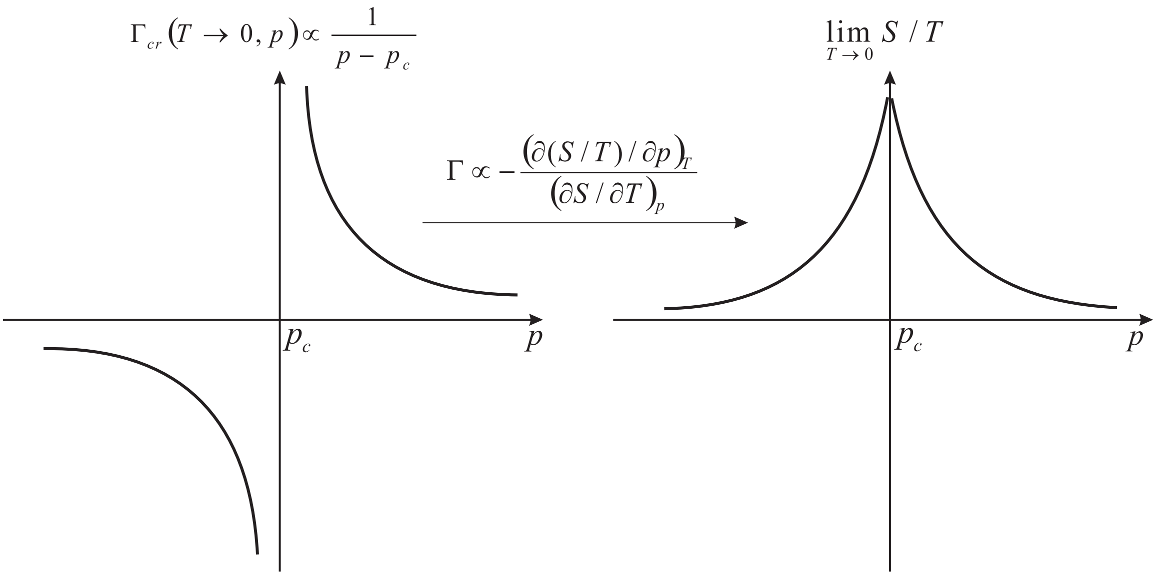

Figure 1. Divergence of the Grüneisen ratio and the accumulation of entropy near QCPs.

2. One-dimensional transverse field Ising model

Consider first the one-dimensional transverse field Ising model (1D TFIM), defined by the Hamiltonian [7]:

$$H_I = -J \sum_i \left(g\hat{\sigma}_i^x + \hat{\sigma}_i^z \hat{\sigma}_{i+1}^z \right), \tag{1}$$

where $J > 0$ is the ferromagnetic Ising coupling between the neighboring spins and gJ is the transverse magnetic field. With the tuning of g, there exists a quantum phase transition from a ferromagnet to quantum paramagnet at $g_c = 1$ [7, 8]. Using a Jordan-Wigner transformation, we can represent the Hamiltonian in the thermodynamic limit in terms of free fermions and the free energy can be written as $F = -Nk_BT \left[\ln 2 + \frac{1}{\pi}\int_0^\pi d\,k \ln\cosh(\varepsilon_k/2k_BT)\right]$, with the dispersion $\varepsilon_k = 2J\left(1 + g^2 - 2g\cos k\right)^{1/2}$. The normalized free energy density is

$$f \equiv \frac{F}{NJk_B} = f_0(g) - \frac{t}{\pi}\int_0^\pi dk \ln\left(1 + e^{-2A}\right); A = \sqrt{(1-g)^2/t^2 + 4(g/t^2)\sin^2(k/2)} \tag{2}$$

where $t = k_BT/J$, and $f_0(g)$ is the ground state energy. Our focus will be on the T-dependent part, $f_1(g,T) = f(g,T) - f_0(g)$.

Consider first the quantum critical regime, where $|g-1|/t \ll 1$. At temperatures small compared to J, we can introduce a momentum cutoff $k_c \approx t$, below which $|\sin(k/2)|/t \ll 1$ and therefore $A \ll 1$. The free energy can be approximated by the contributions from $k < k_c$, which

is

$$f_1 \approx -\frac{t}{\pi}\left[\frac{1}{2}\left(\frac{1-g}{t}\right)^2 k_c + \frac{g}{t^2}\frac{k_c^3}{6} + k_c \ln 2\right] \overset{k_c \approx t}{\approx} -\frac{t^2}{\pi}\left(\left(\frac{g}{6} + \ln 2\right) + \frac{1}{2}\left(\frac{1-g}{t}\right)^2\right) . \quad (3)$$

While Eq. (3) contains approximations for the regular pieces, it reveals an important point. Compared with the general hyperscaling form, this expression is particular in that the linear term $|1-g|/t$ in the expansion vanishes. As a result, the magnetic Grüneisen ratio as a function of temperature at the QCP stays finite.

Consider next the low-temperature regions where $|1-g|/t \gg 1$. Here $A \gg 1$ and we can expand $\ln(1+e^{-2A})$ as e^{-2A} and obtain

$$f_1 \approx -\frac{t^2}{\sqrt{2\pi g}}\left(\frac{|1-g|}{t}\right)^{1/2} e^{-\frac{2}{t}|1-g|} . \quad (4)$$

We can further replace $1/\sqrt{g}$ by $1/\sqrt{g_c}$ without missing any singularity. The free energy has the exact hyperscaling form with $z=1$. We obtain the magnetic Grüneisen ratio to be

$$\Gamma = \frac{1}{g-1} , \quad (5)$$

which is indeed divergent at the QCP, $g_c = 1$. The accumulation of entropy immediately follows (Fig. 1).

3. Spin-density-wave quantum critical point

Quantum phase transitions in itinerant magnets are traditionally described in terms of a $T=0$ spin-density-wave (SDW) transition and formulated as a quantum Ginzburg-Landau theory with dynamic exponent $z > 1$ [9]. For concreteness, we take the 3D antiferromagnetic case as an example, *i.e.*, with $d=3$ and $z=2$. The effective dimension of the Ginzburg-Landau theory is $d+z$, which is above the upper critical dimension 4. Correspondingly, the quartic coupling u, appearing in the action as $u\int \phi^4$, is irrelevant in the renormalization-group (RG) sense. Under the RG transformation, u renormalizes to zero as the fixed point is reached, leaving only the Gaussian (quadratic) part. However, u is dangerously irrelevant [10, 11]. For instance, in the quantum critical regime, the correlation length is determine as $\xi^{-2} \sim r(T) = r + cuT^{3/2}$ (where c is a constant, $4(n+2)(1/3 - \ln 2\sqrt{2}/(3\pi^3))$, with n being the number of components of the order parameter). One can consider u as introducing a new energy scale, and the scaling functions for generic physical quantities are expressed in terms of two variables $f(r/T, uT^{3/2}/r)$.

Within the RG approach [10], it is natural to focus on the free energy associated with the Gaussian term, F_G. The expression for F_G in the RG approach can be shown to be equal to a Gaussian free energy with r replaced by renormalized $r(T)$. We will focus on the quantum critical regime, and write $F_G = F_G^{(1)} + F_G^{(2)}$, where

$$F_G^{(1)} = -nV\int_0^{\Lambda}\frac{d^3q}{(2\pi)^3}\int_0^{\Gamma_q}\frac{d\varepsilon}{2\pi}\left(\coth\frac{\varepsilon}{2T} - 1\right)\tan^{-1}\frac{\varepsilon/\Gamma_q}{r(T) + (q/\Lambda)^2} , \quad (6)$$

and

$$F_G^{(2)} = -nV\int_0^{\Lambda}\frac{d^3q}{(2\pi)^3}\int_0^{\Gamma_q}\frac{d\varepsilon}{2\pi}\tan^{-1}\frac{\varepsilon/\Gamma_q}{r(T) + (q/\Lambda)^2} . \quad (7)$$

Here, $\Gamma_q = \Gamma_0 q^{z-2}$, while Λ and Γ_0 are respectively the ultraviolet momentum and energy cutoffs. The leading temperature-dependent contribution from $F_G^{(2)}$ turns out to be $\frac{nV\Lambda^3\Gamma_0}{4\pi^3}\left(\frac{\sqrt{2}\pi}{4} + \ln 2 - \frac{\sqrt{2}}{2}\ln(\sqrt{2}+1)\right) c(u/\Gamma_0^{3/2})T^{3/2}$, which is more singular than that from $F_G^{(1)}$.

This Gaussian form, however, is incomplete. The quartic coupling also introduces an explicitly linear in u term ($t \equiv T/\Gamma_0$), which takes the form

$$F_u = -2n(n+2)N\Gamma_0 u \int_0^\infty e^{-6x} \left(\int_0^1 \frac{d^3q}{(2\pi)^3} \int_0^1 \frac{d\varepsilon}{\pi} \coth \frac{\varepsilon}{2te^{2x}} \frac{\varepsilon}{\varepsilon^2 + (re^{2x} + q^2)^2} \right) f_u \, dx \, ,$$
$$f_u \equiv \frac{1}{2\pi^2} \int_0^1 \frac{d\varepsilon}{\pi} \coth \frac{\varepsilon}{2te^{2x}} \frac{\varepsilon}{\varepsilon^2 + (re^{2x} + 1)^2} + \frac{2}{\pi} \int \frac{d^3q}{(2\pi)^3} \coth \frac{1}{2te^{2x}} \frac{1}{1 + (re^{2x} + q^2)^2} \, . \quad (8)$$

We find that, to the linear order in u, the leading temperature-dependent contribution from F_u exactly cancels that of $F_G^{(2)}$, leaving the singular contribution to the total free energy to be

$$F_{tot} \approx F_G^{(1)} \, , \quad (9)$$

which is given by

$$F_{tot} \sim -2\frac{T^2}{\Gamma_0^2} + \frac{2\pi T^{5/2}}{\Gamma_0^{5/2}} \left(1 + \frac{9}{2} \frac{r + cuT^{3/2}/\Gamma_0^{3/2}}{T/\Gamma_0} \right) \, . \quad (10)$$

We can trace the singular terms included in Eq. (6) to the contributions of the low-energy degrees of freedom, and those included in Eq. (7) to a unphysical origin from the degress of freedom at high energies and short distances near the cutoff scales. Eqs. (6,9) are therefore expected to be the regularization prescription that is valid to all orders in u. The explicit result given in Eq. (10) is consistent with those often quoted in the literature. The T^2 term represents the background Fermi liquid contribution. The critical part of the free energy is consistent with the scaling form $T^{5/2}(1 + r/T)$. The contribution of the renormalized quartic coupling $uT^{3/2}$ to the free energy is subleading; the dangerously irrelevant parameter does not modify the leading singular part of the free energy from its hyperscaling form, thereby preserving the divergence of the Grüneisen ratio and the accompanied entropy accumulation.

4. Summary
We have considered the thermodynamic properties of two models of quantum criticality. We have analyzed the potential effects beyond the most general hyperscaling forms in both models, and established that entropy accumulation is a robust property of both models.

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